Validity and limitations of the detection matrix to determine hidden units and network size from perceptible dynamics

Maurizio Porfiri*
Department of Mechanical and Aerospace Engineering and Department of Biomedical Engineering, New York University, Tandon School of Engineering, Brooklyn, New York 11201, USA
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Determining the size of a network dynamical system from the time-series of some accessible units is a critical problem in network science. Recent work by Haehne *et al.* [1] has presented a model-free approach to address this problem, by studying the rank of a detection matrix that collates sampled time-series of perceptible nodes from independent experiments. Here, we unveil a profound connection between the rank of the detection matrix and the control-theoretic notion of observability, upon which we conclude when and how it is feasible to exactly infer the size of a network dynamical system.

Introduction. From natural to technological settings, network dynamical systems constitute a powerful approach to study collective dynamics [2–4]. Within this modeling scheme, each network node is associated with an individual dynamical system and each link encapsulates the interaction between two coupled units. Fueled by the increasing availability of massive datasets, the theory of network dynamical systems promises to unveil the underpinnings of complexity [5].

Toward achieving this ambitious goal, considerable effort is being placed to establish effective methodologies to build network representations from time-series of individual units. Through advancements in statistically-principled network reconstruction, neuroscientists can tackle the inference of functional connectivity patterns in the brain from electroencephalography data [6], Earth scientists can utilize weather data to pinpoint causal links underlying the climate [7], and biologists can track animals' motion to unveil social structures behind collective behavior [8].

Pervasive to most of these efforts is the assumption that the researcher has complete access to all the nodes in the network. However, seldom do we possess full knowledge about the dynamics of the system, since many of the units are hidden from measurements. Hence, the process of network inference could be hindered by the presence of hidden nodes that would confound the dynamics of accessible units. For example, should one be interested in the organization of a migrating fish school [9], they must rely on measurements of only a few tagged individuals: the vast majority of the school will not be measurable. In fact, the researcher may not even know how many individuals compose the school.

Detecting the number of hidden nodes from a few perceptible nodes was the open question addressed in Ref. 1. Therein, the authors put forward a promising model-free approach to estimate the true network size from the rank of a detection matrix that comprises the sampled time-series of perceptible nodes from independent experiments. Here, we uncover deep roots of this model-free approach in the classical theory of control systems by Kalman [10]. Upon these roots, we rigorously study the inner workings of the detection matrix to determine when and how it is feasible to exactly infer the size of a network dynamical system. Our results demonstrate that the seemingly distinct challenges of identifying the number of units in a network from perceptible nodes and reconstructing the state of the whole network from them are, in fact, intertwined.

Detecting hidden nodes and network size. We consider a network of N dynamical systems described by a vector function $F:\mathbb{R}^N \to \mathbb{R}^N$, such that

$$\dot{x}(t) = F(x(t)), \tag{1}$$

where $x(t) = [x_1(t), \cdots, x_N(t)]^{\mathrm{T}}$ collates the scalar states of all the nodes, F encodes both the dynamics of the individual units and their interconnecting network, and $t \in \mathbb{R}^+$ is time. Given an ensemble of M measurements, each sampled at k consequent times $t_1, \ldots, t_k$ for n perceptible nodes, can we infer that there are other $N - n$ hidden nodes?

The approach of Ref. 1 is based on the detection matrix

$$T_{(k,M)} = \begin{bmatrix} y^{(1)}(t_1) & \cdots & y^{(M)}(t_1) \\ \cdots & \cdots & \cdots \\ y^{(1)}(t_k) & \cdots & y^{(M)}(t_k) \end{bmatrix}, \tag{2}$$

where $y^{(m)}(t) \in \mathbb{R}^n$ is the measurement vector formed by the time-evolution of the n perceptible nodes during the m-th experiment. For a sufficiently large number of experiments and time-samples, the authors proposed that the rank of $T_{(k,M)} \in \mathbb{R}^{kn\times M}$ is an estimate of N. Through extensive numerical simulations, they find that the method works reliably on several synthetic and experimental networks of coupled dynamical systems, linear or nonlinear.

An example where the method fails. To illustrate the roots of the detection matrix in mathematical control theory, we consider an undirected, unweighted path graph of $N = 3$ nodes, such that 1 is the center and 2 and 3 are the terminals. Let the three nodes implement a linear consensus algorithm [11], where each of them averages its state with its neighbors according to

$$\dot{x}(t) = -Lx(t), \tag{3}$$

with L being the Laplacian matrix [12], that is, $L = \begin{bmatrix} 2 & -1 & -1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix}$. If only node 1 is perceptible, we could only measure a sampled version of $x_1(t)$, which, upon integrating (3), reads

$$x_1(t) = \frac{1}{3}\left(2e^{-3t}+1\right)x_{10} + \frac{1}{3}\left(1-e^{-3t}\right)(x_{20}+x_{30}), \tag{4}$$

where x_{10}, x_{20}, and x_{30} are the initial conditions.

By sampling the time-evolution of this perceptible node at k times and considering M experiments associated with initial conditions $x_0^{(1)}, \ldots, x_0^{(M)}$, we construct the detection matrix in (2). Irrespective of how large M and k are, it is impossible to find three columns of the detection that are linearly independent. The initial conditions of nodes 2 and 3 enter the evolution of the perceptible node only via their summation, thereby leaving undistinguishable footprints on the evolution of node 1. In this case, the rank of the detection matrix will converge to two and the method will incorrectly suggest that there is only one hidden node. To produce three independent columns in the detection matrix and infer the exact network size, we should require that nodes 2 and 3 separately enter the evolution of node 1.

The mathematical backdrop to formulate general conditions for the successful application of the detection matrix should be sought in the notion of observability, formulated by Kalman more than fifty years ago [10] to examine the problem of reconstructing unmeasurable state variables from measurable ones. Several recent studies within the control community [13–19] have studied observability of network dynamical systems, but they assumed complete knowledge of the system dynamics. Here, we seek to lay the mathematical foundations for the fundamental question posed in Ref. 1, that is, to detect hidden units and network size from a detection matrix assembled from raw time-series. We focus our mathematical treatment on linear time-invariant (LTI) systems, like the consensus problem in (3) – analysis of linear time-varying systems is included in the Supplemental Material [20].

Theory. For a LTI system with state matrix A, the state transition matrix $\Phi(t,0)$ that maps the initial state vector x_0 to its value at t is given by the matrix exponential [21], that is, $\Phi(t,0) = e^{At}$. The computation of the matrix exponential can be carried out in a number of ways [22]. One possibility is to apply Cayley-Hamilton theorem that states that every square matrix satisfies its own characteristic equation [22], thereby implying that any power of A higher than N can be written as a linear combination of lower powers, from 0 to $N-1$. Since the matrix exponential is an analytic function that can be written in Taylor series, we establish

$$\Phi(t,0) = \sum_{j=0}^{N-1} \alpha_j(t) A^j, \tag{5}$$

where $\alpha_0(t), \ldots, \alpha_{N-1}(t)$ are unknown analytic time-functions that can be written in terms of the spectrum of A.

Assuming for simplicity that all the eigenvalues of A are distinct, we can project (5) on each of the eigenvectors of A to obtain the following linear system for $\alpha_0(t), \ldots, \alpha_{N-1}(t)$ [23]:

$$e^{\lambda_i t} = \sum_{j=0}^{N-1} \alpha_j(t) \lambda_i^j, \tag{6}$$

for $i = 1, \ldots, N$, where $\lambda_1, \ldots, \lambda_N$ are the complex eigenvalues of A. By introducing vectors $\alpha(t) = [\alpha_0(t), \cdots, \alpha_{N-1}(t)]^{\mathrm{T}} \in \mathbb{R}^N$ and $E(t) = [e^{\lambda_1 t}, \cdots, e^{\lambda_N t}]^{\mathrm{T}} \in \mathbb{C}^N$, we can write (6) in the compact matrix form $E(t) = V\alpha(t)$, where $V \in \mathbb{C}^{N\times N}$ is the Vandermonde matrix constructed from the eigenvalues of A. The j-th column of the Vandermonde matrix is $\left[\lambda_1^{j-1}, \cdots, \lambda_N^{j-1}\right]^{\mathrm{T}}$. Given that the eigenvalues are distinct, V is invertible and its determinant is equal to $\prod_{1\le i<j\le N}(\lambda_j - \lambda_i)$ [24].

Without loss of generality, we assume that the first n network nodes are the perceptible ones, so that the output matrix of the LTI system is $C = [I_{nn}, 0_{n(N-n)}]$, where I_{nn} is the identity matrix in $\mathbb{R}^{n\times n}$ and $0_{n(N-n)}$ is the zero matrix in $\mathbb{R}^{n\times(N-n)}$. From (5), the time-evolution of the perceptible nodes is

$$y(t) = Cx(t) = \sum_{j=0}^{N-1} \alpha_j(t) \mathcal{O}_j x_0, \tag{7}$$

where we have introduced the matrices $\mathcal{O}_j = CA^j$ to form the so-called [21] observability matrix $\mathcal{O} = [\mathcal{O}_0^{\mathrm{T}}, \ldots, \mathcal{O}_{N-1}^{\mathrm{T}}]^{\mathrm{T}} \in \mathbb{R}^{nN\times N}$. The observability matrix of an LTI system maps the initial condition to the vector collating the time-derivatives of the output at the initial time, up to the order $(N-1)$, thereby quantifying the extent by which the internal dynamics of the network can be observed from its perceptible nodes.

For the assembly of the detection matrix in (2), we must sample $y(t)$ at k different times – for simplicity, we assume that these times are equidistant at a sampling period Δt, such that $t_s = (s-1)\Delta t$ with $s = 1, \ldots, k$. Hence, we determine the following compact form for the detection matrix:

$$T_{(k,M)} = \left[\alpha_{(k)} \otimes I_{nn}\right] \mathcal{O} X_0, \tag{8}$$

where $\otimes$ is the Kronecker product [21], $X_0 = [x_0^{(1)}, \cdots, x_0^{(M)}] \in \mathbb{R}^{N\times M}$, and $\alpha_{(k)} \in \mathbb{R}^{k\times N}$ collates the sampled values of the coefficients in the Cayley-Hamilton expansion. By using (6), we express each row of the matrix $\alpha_{(k)}$ in terms of the samples of $E(t)$, yielding

$$\alpha_{(k)} = E_{(k)}^{\mathrm{T}} V^{-\mathrm{T}}, \tag{9}$$

where $E_{(k)} \in \mathbb{R}^{N\times k}$ is such that its s-th column is $E(t_s)$.

Two hypotheses on the quantity and quality of the perceptible dynamics are needed to ensure that the rank of the detection matrix could be informative of the size of the network, or, at least, part of it. First, we should have at least N time-samples, that is, $k \geq N$. Under this assumption and given that we are focusing on equidistant samples, the first N columns of $E_{(k)}$ constitute a nonsingular Vandermonde matrix, implying that $E_{(k)}$ is full row rank [25]. Second, we should have $M \geq N$ to obtain N independent experiments, such that X_0 is full row rank.

Before we proceed, we recall three classical matrix properties [24, 26]. Given two conforming matrices A and B: first, if A is full column rank, then $\mathrm{rank}(AB) = \mathrm{rank}(B)$; second, if A is full row rank, then $\mathrm{rank}(BA) = \mathrm{rank}(B)$; and third, $\mathrm{rank}(A\otimes B) = \mathrm{rank}(A)\mathrm{rank}(B)$. By recalling that V is invertible, the second property implies that $\mathrm{rank}\left(\alpha_{(k)}\right) = \mathrm{rank}\left(E_{(k)}^{\mathrm{T}}\right)$; given that $E_{(k)}$ is full row rank, then $\alpha_{(k)}$ is full column rank. By virtue of the third property, the Kronecker product in (8) constitutes a full column rank matrix and application of the first property implies that $\mathrm{rank}\left(T_{(k,M)}\right) = \mathrm{rank}\left(\mathcal{O}X_0\right)$. Finally, by recalling that X_0 is full row rank, application of the second property leads to our main claim,

$$\mathrm{rank}\left(T_{(k,M)}\right) = \mathrm{rank}(\mathcal{O}). \tag{10}$$

Hence, monitoring the rank of the detection matrix helps estimating the rank of the observability matrix of the associated LTI system, which is equal to the size of the network if and only if the LTI system is (completely) observable [21]. If the system is not observable, the rank of the detection matrix provides an estimate of the dimension of the largest observable subset of the system, based on Kalman decomposition [21]. The latter consists of a coordinate transformation that decomposes the dynamics into an observable and an unobservable component. In the transformed block-triangular structure of the system, all the measurements are performed on the observable component, which evolves independently of the unobservable one.

Analogous claims to (10) can be derived for linear time-varying systems, associated with time-varying topologies and node dynamics; see Supplemental Material. The main difference is that the length of the time-series could be much longer than the network size to ensure convergence of the rank of the detection matrix to the exact network size for observable systems.

Application of the theory to consensus problems. With respect to the earlier example of a three-node path graph, the observability matrix is $\mathcal{O} = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 1 \\ 6 & -3 & -3 \end{bmatrix}$. The rank of $\mathcal{O}$ is equal to two, consistent with what we could discover from the detection matrix. Should we have access to any of the terminals, rather than the center, $\mathcal{O}$ would have rank equal to three and the detection matrix will help discover the true size of the network. In this case, the initial conditions of non-perceptible nodes would separately enter the evolution of the perceptible one, different from (4).

Even without access to the terminals, the three-node graph is observable from its center if we weighted the links by two unequal, nonzero constants w_{12} and w_{13}, since $|\det(\mathcal{O})| = |w_{12}w_{13}(w_{12} - w_{13})| \neq 0$ [27]. Likewise, introducing time-varying patterns in the interaction between the nodes can facilitate observability by modulating the effect of hidden nodes on the perceptible dynamics. As shown in the Supplemental Material, it is possible to design periodic temporal patterns that will ensure observability of the path graph, even though the corresponding time-average network would describe an unobservable LTI system.

Criteria for observability of undirected, unweighted path graphs of arbitrary size have been formulated in Ref. 17. Interestingly, only path graphs with 2^q nodes, with q being a positive integer, are observable from any node, thereby supporting the exact inference of the network size from any choice of perceptible nodes. For any other path graph, unless we have access to one of the two terminals [16], the rank of the detection matrix could underestimate the exact network size [28]. Similar claims are gathered for undirected, unweighted cycle graphs [17], where observability is achieved by accessing two adjacent nodes or even any two nodes if N is a prime number, but never via a single node.

The study of observability of path and cycle graphs indicate some of the drawbacks in the application of the detection matrix to networks with homogeneous degree distribution. A much more dramatic scenario is noted when dealing with star networks, where the detection matrix may be of no practical use. In fact, for an undirected, unweighted star of N nodes, observability requires access to at least $N-2$ of the terminals, so that correctly estimating the network size from the detection matrix requires accessing all but two nodes. The proof of this claim is based on the Popov-Belevich-Hautus lemma [21], which states that an LTI system is unobservable if and only if A has an eigenvector w in the null space of C.

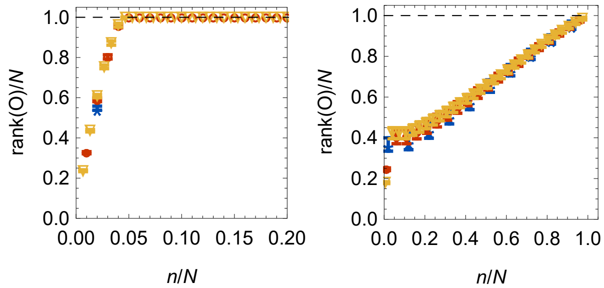
Specifically, the state matrix is symmetric [12], with eigenvalues N and 0 of multiplicity 1, and 1 with multiplicity $N-2$. Taking node 1 as the center, the eigenvector corresponding to the largest eigenvalue is $w_N = [N-1, -1, \cdots, -1]^{\mathrm{T}}$, the one corresponding to the smallest one is $w_1 = [1, \cdots, 1]^{\mathrm{T}}$, and the eigenspace corresponding to the unit eigenvalue is $W_2 = \mathrm{Span}\{w_1, w_N\}^{\perp}$. For any choice of $n \leq N-2$ perceptible nodes in the star that includes the center, there is always $w \neq 0$ in W_2, which has zero components in correspondence to all the perceptible nodes. If the center is not part of the perceptible dynamics, any choice of $n \leq N-3$ perceptible nodes would lead to the existence of some $w \neq 0$ in W_2 with zero components in correspondence to any perceptible node [29].

Dealing with random networks, we reach the same conclusions, whereby the inference of the size of heterogenous networks from the detection matrix could not be practically viable. We illustrate this claim by studying two unweighted directed random graphs with average out-degree $\lfloor N/10 \rfloor$: the homogeneous random graph considered in Ref. 1 and a heterogenous random graph obtained by adapting the version of the Barabási-Albert [30] algorithm proposed in Ref. 31. The algorithm starts from a complete network of $\lfloor N/10 \rfloor + 1$ nodes and iteratively adds new nodes in a sequence of steps, which are preferentially attached to high in-degree nodes, maintaining an almost constant out-degree distribution.

Figure 1 shows that access to less than 10% of the nodes is sufficient to exactly infer the network size ($\mathrm{rank}(\mathcal{O}) = N$) of a homogeneous network, which is in line with numerical evidence by Ref. 1, but reliably estimating the size of a heterogeneous network is unfeasible. While the standard deviations in the rank of the detection matrix are negligible for the homogeneous network, we record standard deviations as large as 5% for heterogeneous networks. Hence, the selection of the perceptible nodes has negligible influence on the accuracy of the inference for homogeneous networks, while it can play a critical role for heterogeneous networks. This evidence is in agreement with our analysis of star graphs, which supports that access to the center is less important than access to terminal nodes, and with results in Ref. 16, which pinpoint at a mediating effect of local connectivity on network observability in star-shaped networks.

These findings confirm that caution is warranted when drawing inference regarding the size of a network from the dynamics of perceptible nodes, unless one has some prior knowledge regarding the network dynamical system. Practically, we can only attempt at estimating the size of the largest observable subset of the network dynamical system, which could be only a small portion of the whole system. For consensus protocols over unweighted networks, heterogeneity has a detrimental effect on observability, whereby access to most of the network nodes is required for accurately inferring the network size.

Conclusion. Technical progress in the theory of network dynamical systems has often been informed by mathematical control theory. For example, the study of synchronization of chaotic oscillators has benefitted by a strong connection with the theory of Lyapunov stability



(a) (b)

FIG. 1. Rank of the observability matrix of (a) homogenous and (b) heterogenous directed random networks of N nodes, executing the consensus protocol in (3), as a function of the fraction of perceptible nodes n/N, for $N = 50$ (blue squares), $N = 100$ (open red circles), and $N = 150$ (orange triangles). Simulations are average values over 100 runs and error bars indicate standard deviations. The black dashed line indicates perfect inference of the network size.

[32], which allows for the formulation of a master stability function that clarifies the interplay between individual dynamics and network topology on synchronization. Likewise, the notions of controllability and controllability Gramian have clarified the possibility of steering the evolution of a network dynamical system toward desired states through control actions at a few selected nodes [33, 34].

We propose that the relationship between the detection matrix [1] and the concept of observability uncovered in this work could beget similar methodological and theoretical advances. This paper shows that the success of the detection matrix in exactly estimating the size of a network is, in fact, conditional to the complete observability of the system from its perceptible dynamics. Irrespective of the number of independent experiments and the number of samples, any inference based on measurable nodes is limited to the observable portion of the network dynamical system.

The observable portion of the network dynamical system could be a small portion of the entire system when dealing with networks of heterogeneous degree distribution. For example, while one or two perceptible nodes would be sufficient to exactly estimate the size of an unweighted path graph, all but two of the nodes must be accessed when attempting to infer the size of an unweighted star graph executing a consensus protocol. Likewise, working with consensus over random networks, a few randomly selected nodes may be sufficient for the inference of homogeneous networks, but access to almost all the nodes could be needed for heterogeneous networks. Hence, prudence is recommended in the application of the approach to several domains of investigation where heterogeneous networks are pervasive, such as social, transportation, and sociotechnical systems [35]. Interestingly, temporal patterning of the network connections might facilitate observability and improve the power of the detection matrix, by enhancing differences in the footprint of hidden nodes on the perceptible dynamics.

From the perspective of control theory, the correspondence between the detection matrix and the concept of observability could be leveraged in other applications, where one has knowledge of the network size, but not about the dimension of its largest observable subset. In this vein, it may be possible to establish model-free strategies to study observability of networks from the detection matrix. These model-free strategies could complement existing methodologies to reconstruct network structure from time-series [36, 37] and discover model equations [38], facilitating the study of critical control-theoretic metrics from data.

Upon the discovered connection between the detection matrix and network observability, one may pursue several lines of further inquiry. In its present formulation, the approach assumes that each network node has a scalar dynamics, so that the dimension of the largest observable set corresponds to the network size. It is paramount to establish model-free techniques for inferring the size of networks whose nodes have vectorial dynamics, potentially of different order. In addition, the mathematical treatment presented herein is based on a linear, analytic model for the network dynamical system, which might not be valid in many applications across natural and technological settings where nonlinearities, nonsmoothness, and stochasticity cannot be discarded.

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* Author for correspondence (mporfiri@nyu.edu)

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[28] For example, a path graph of six nodes is not observable from the two internal nodes that are adjacent to the terminals [17].
[29] For example, in a star graph of six nodes where we have access to nodes 2, 3, and 4, $w = [0, 0, 0, 0, 1, -1]^{\mathrm{T}}$ belongs to the eigenspace corresponding to the unit eigenvalue and is in the null space of C. Had we access to the center of the star, w would still be in the null space of C, but, had we included an extra terminal, say node 5, w would not be in the null space of C.
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